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An Anti-WKB Approximation

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Abstract

In the WKB approximation the $\nabla^2 S$ term in Schrödinger's equation is subordinate to the $|\nabla S|^2$ term. Here we study an *anti-WKB approximation* in which the $\nabla^2 S$ term dominates (after a guess for S is supplied). Our approximation produces only the nodeless ground state wavefunction, but it can be used in potential problems where the potential is not symmetric, and in problems where there are many degrees of freedom. As a test, we apply the method to potential problems, including the hydrogen and helium atoms, and to ϕ^4 field theory.

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1 Introduction

In quantum mechanics the wavefunction is sometimes written in the form

$$\psi(\mathbf{r}) = \exp S(\mathbf{r}). \quad (1.1)$$

Schrödinger's equation then takes the form

$$\nabla^2 S + |\nabla S|^2 = \frac{2m}{\hbar^2} [V(\mathbf{r}) - E]. \quad (1.2)$$

The WKB approximation ensues when the term $\nabla^2 S$ is dropped in leading order and later incorporated as a correction.[1] It is commonly understood that this step is justified in the semi-classical regime where the gradient of the de Broglie wavelength, $\nabla\lambda$, has a magnitude much smaller than one, and the wave function oscillates many times over distances that characterize the variation of the potential.

In this paper we consider the alternate ordering of terms where the term $|\nabla S|^2$ is dropped in leading order and later treated as a correction. This is an *anti-WKB approximation*. As we shall see, the anti-WKB approximation is valid deep in the quantum regime where the wavefunction is nodeless and therefore changes over a length that is at least as great as that which characterizes the variation of the potential. For a particle moving in a potential, such a wavefunction describes a bound state. In a bosonic field theory it describes the ground state.

The anti-WKB approximation is not as straightforward as the WKB approximation because it is not generally true that $|\nabla^2 S| \gg |\nabla S|^2$ for bound state wavefunctions. To see this explicitly, assume the potential vanishes when $r > a$. Then for $r > a$,

$$S = S_0 - Kr - \frac{D-1}{2} \ln(r/r_0); \quad K \equiv \sqrt{-\frac{2mE}{\hbar^2}}, \quad (1.3)$$

where motion is in D spatial dimensions. Comparing the gradient and Laplacian applied to this expression, we find that the anti-WKB approximation is justified only when $D = 1$ and $K = 0$ (or at least $K \sim 0$.) This is the case of a weakly bound particle moving in one dimension. (Recall that in one dimension there is always one bound state in an attractive potential, no matter how weak the potential.) This version of the anti-WKB approximation has

been developed.[2] One obtains an expression for the energy of the bound state as a series of integrals over powers of the potential. The relative size of the n -th term is proportional to the n -th power of the parameter $V_0 m a^2 / \hbar^2$, where V_0 is the strength of the potential and a its range. We see here an expected contrast with the WKB approximation: a series of *decreasing* powers of Plack's constant. Despite this, if the potential is such as to make the parameter small, the approximation succeeds.

The straightforward case just described is quite different from the anti-WKB approximation considered in this paper, where we treat the general case $D \neq 1$, $K \neq 0$. We evade the “no-go” conclusion, above, by supplying an initial guess for S . Thus we write

$$S(\mathbf{r}) = F(\mathbf{r}) + T(\mathbf{r}), \quad (1.4)$$

where the variational seed F has the asymptotic form 1.3, and is chosen to be an initial guess for S . The correction T is now determined by Schrödinger's equation:

$$\nabla^2 T_n + 2\nabla F \cdot \nabla T_n = \frac{2m}{\hbar^2} [V(\mathbf{r}) - E_n] - \nabla^2 F - |\nabla F|^2 - |\nabla T_{n-1}|^2; \quad T_{-1} = 0. \quad (1.5)$$

The index $n = 0, 1 \dots$ labels the successive approximations to T and hence S . The initial approximation ignores the gradient of T ; the next approximation uses the initial approximation for the gradient, and so forth. Of course, ignoring the gradient of T is different than ignoring the gradient of S , much of which appears in Eq. 1.5 in the term $|\nabla F|^2$; nevertheless, we still call this the anti-WKB approximation. Note that for each n we obtain a different approximation for the bound state energy, E_n .

In Section 2 we demonstrate that this sequence of approximations is formally convergent provided F is well chosen. It is useful to state what we find. Assume that our variational seed differs from S by a function scaled by a small parameter ϵ :

$$F(\mathbf{r}) = S(\mathbf{r}) - \epsilon S_1(\mathbf{r}). \quad (1.6)$$

It follows that the exact T is ϵS_1 . In Section 2 we show that

$$E_n = E + \epsilon^{n+2} A_n; \quad T_n = \epsilon S_1 + \epsilon^{n+2} R_n. \quad (1.7)$$

Here E is the true bound state energy, and the factors A_n and R_n are finite at $\epsilon = 0$. The convergence is formal because we have not given estimates for the n -dependence of A_n and R_n . If these factors increase with n faster than an exponential, the sequence does not converge, but is instead asymptotic.

The convergence estimates of Eq. 1.7 depend on the fact that the term T_{n-1} appears quadratically on the right hand side of Eq. 1.5. When F differs little from S , treating the gradient as a correction is justified. We again emphasize the difference between what is done in Ref. [2] and what we do here. This is not a weak potential approximation, nor is it an expansion in inverse powers of \hbar . We rely on the availability of a reasonable guess for the variational seed F . The guess must also be such that the integrals and Green functions we shall encounter can be computed.

The wavefunction arising from our construction is nodeless. The reason is that if ψ vanishes on the surface $f(\mathbf{r}) = 0$, there will be a term $\ln f(\mathbf{r})$ in S . In the neighborhood of the node, this logarithm dominates S , and we must explicitly incorporate it into F if we are to obtain a wave function with a node. Note that we must specify the surface $f = 0$, which is known only under special circumstances. We do not consider such cases here; our F 's will be smooth, and we therefore limit ourselves to nodeless wavefunctions. This means that the energies E_n are approximations to the ground state energy E .

Like the WKB approximation, the anti-WKB approximation is nonperturbative; it does not require the presence of a small parameter in the Hamiltonian. Its major limitation is that it is restricted to the ground state wave function. But the anti-WKB approximation has this important advantage: Equation 1.5 for T_n is linear. We will see that it can be solved readily in many cases of interest, including particles moving in three dimensions in asymmetric potentials, and many-body problems like bosonic lattice field theory. In the latter problem the method can be extended to study some of the vacuum state correlation functions that are of central importance in field theory. All these possibilities are closed to the WKB approximation, which is generally unmanageable except for a particle whose motion effectively reduces to one dimension. It should be noted that the anti-WKB approximation is less useful for problems involving identical fermions because the Pauli principle makes the nodeless state unphysical for systems of more than two spin 1/2 particles.

In Section 2 we present a theoretical development of the anti-WKB ap-

proximation. We include the solution of the dynamical equation 1.5, the convergence of the sequence of approximations, and several other matters.

In following sections the anti-WKB approximation is applied to a number of problems to show that it works in increasingly complex situations. In Section 3 we study a spherically symmetric square well whose ground state is known by elementary methods. We find that E_0 gives only 62% of the correct binding energy, but the next approximation, E_1 , gives 96%. We develop Green functions required for the application of Eq. 1.5 to potential problems where the potential is nonspherical. In Section 4 we study long range potentials, with the hydrogen atom as a particularly simple subcase. We finish by applying the anti-WKB approximation to many-body problems: ϕ^4 field theory in Section 5, and the helium atom in Section 6. Conclusions are presented in Section 7.

2 Anti-WKB Equations

The energies in Eq. 1.5 are determined by a general requirement. Consider the surface integral

$$\oint_S d\mathbf{A} \cdot [e^{2F} \nabla T_n] = \int_V dV \nabla \cdot [e^{2F} \nabla T_n]. \quad (2.1)$$

As S is expanded to infinity, the surface integral decreases to zero because of the exponential fall of the factor e^{2F} . Using Eq. 1.5 we obtain the eigenvalue equation determining E_n :

$$0 = \int dV e^{2F} \left\{ \frac{2m}{\hbar^2} [V(\mathbf{r}) - E_n] - \nabla^2 F - |\nabla F|^2 - |\nabla T_{n-1}|^2 \right\}. \quad (2.2)$$

We can now assemble the equations to derive the convergence results 1.7. The true ground state energy E is determined by Eq. 2.2 with the replacements $E_n \rightarrow E$, $T_{n-1} \rightarrow T$. Subtracting equations,

$$\begin{aligned} 0 &= \int dV e^{2F} \left[\frac{2m}{\hbar^2} (E_n - E) + |\nabla T_{n-1}|^2 - |\nabla T|^2 \right], \\ E_n &= E + \frac{\hbar^2}{2m} \frac{\int dV e^{2F} [|\nabla T|^2 - |\nabla T_{n-1}|^2]}{\int dV e^{2F}}. \end{aligned} \quad (2.3)$$

We now express the n -th order factors in terms of their limiting values and a deviation:

$$\begin{aligned} E_n &= E + a_n, \\ T_n &= -\epsilon S_1 + r_n. \end{aligned} \quad (2.4)$$

Then Eq. 2.3 becomes

$$\begin{aligned} a_0 &= \epsilon^2 \frac{\hbar^2}{2m} \frac{\int dV e^{2F} |\nabla S_1|^2}{\int dV e^{2F}}, \\ a_n &= \frac{\hbar^2}{2m} \frac{\int dV e^{2F} [2\epsilon \nabla S_1 \cdot \nabla r_{n-1} - |\nabla r_{n-1}|^2]}{\int dV e^{2F}}, \quad (n \geq 1). \end{aligned} \quad (2.5)$$

We next use Eq. 1.5 and the analogous equation for $T = \epsilon S_1$. Subtracting the equations

$$\begin{aligned} \nabla^2 r_0 + 2\nabla F \cdot \nabla r_0 &= -\frac{2m}{\hbar^2} a_0 + \epsilon^2 |\nabla S_1|^2, \\ \nabla^2 r_n + 2\nabla F \cdot \nabla r_n &= -\frac{2m}{\hbar^2} a_n + 2\epsilon \nabla S_1 \cdot \nabla r_{n-1} - |\nabla r_{n-1}|^2. \quad (n \geq 1). \end{aligned} \quad (2.6)$$

It follows that Eq. 1.7 holds for $n = 0$. Furthermore, if 1.7 holds for n , then from Eqs. 2.5, 2.6 we see that it holds for $n + 1$, and the result is established by induction.

Energy E_n requires T_{n-1} for its computation. This information can be used to find a better estimate of the state energy from the expectation

$$\mathcal{E}_n = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle}, \quad \psi = \exp(F + T_{n-1}). \quad (2.7)$$

The error in ψ is $O(\epsilon^{n+1})$; variational argument [3] gives

$$\mathcal{E}_n - E = O(\epsilon^{2n+2}); \quad \frac{\mathcal{E}_n - E}{|E_n - E|} = O(\epsilon^n). \quad (2.8)$$

Eq. 1.5 may be solved using the Green function satisfying

$$\begin{aligned} LG(\mathbf{r}, \mathbf{r}') &= \delta(\mathbf{r} - \mathbf{r}'), \\ L &= \nabla^2 + 2(\nabla F) \cdot \nabla. \end{aligned} \quad (2.9)$$

Then

$$T_n(\mathbf{r}) = \int dV' G(\mathbf{r}, \mathbf{r}') \left\{ \frac{2m}{\hbar^2} [V - E_n] - \nabla^2 F - |\nabla F|^2 - |\nabla T_{n-1}|^2 \right\}_{\mathbf{r}'} . \quad (2.10)$$

It is illuminating to expand the Green function in terms of the orthonormal eigenfunctions of L , because the argument leads to the eigenvalue equation 2.2 in a different way.

$$L\phi_k = \mu_k \phi_k; \quad \int dV e^{2F} \phi_{k1} \phi_{k2} = \delta_{k1,k2}. \quad (2.11)$$

Then

$$G(\mathbf{r}, \mathbf{r}') = \sum_k \frac{1}{\mu_k} \phi_k(\mathbf{r}) \phi_k(\mathbf{r}') e^{2F(\mathbf{r}')} . \quad (2.12)$$

But there is a problem: L annihilates a constant function, so there is a normalized eigenfunction of L with eigenvalue zero:

$$\phi_0(\mathbf{r}) = N, \quad N = \left[\int dV e^{2F} \right]^{-1/2}; \quad \mu_0 = 0. \quad (2.13)$$

The contribution of this zero mode to G is infinite. Nonetheless, T_n in Eq. 2.10 is finite if the projection of the driving term onto the zero mode vanishes. The condition for that is the eigenvalue equation 2.2.

The eigenvalue equation for E_1 can be simplified. We need the integral

$$- \int dV e^{2F} |T_0|^2 = - \int dV \nabla \cdot [e^{2F} T_0 \nabla T_0] + \int dV e^{2F} T_0 \nabla \cdot [e^{2F} \nabla T_0] \quad (2.14)$$

The first integral on the right vanishes by the divergence theorem, and the second may be transformed using Eq. 1.5.

$$- \int dV e^{2F} |T_0|^2 = \int dV e^{2F} T_0 D = \int dV dV' e^{2F(\mathbf{r})} D(\mathbf{r}) D(\mathbf{r}') G(\mathbf{r}, \mathbf{r}'), \quad (2.15)$$

where

$$D \equiv \frac{2m}{\hbar^2} [V - E_0] - \nabla^2 F - |\nabla F|^2. \quad (2.16)$$

The quantization condition for E_1 reads

$$\begin{aligned} 0 &= \int dV e^{2F} \left[D + \frac{2m}{\hbar^2} (E_0 - E_1) \right] + \int dV dV' e^{2F(\mathbf{r})} D(\mathbf{r}) D(\mathbf{r}') G(\mathbf{r}, \mathbf{r}'); \\ E_1 &= E_0 + \frac{\hbar^2}{2m} \frac{\int dV dV' e^{2F(\mathbf{r})} D(\mathbf{r}) D(\mathbf{r}') G(\mathbf{r}, \mathbf{r}')}{\int dV e^{2F}}. \end{aligned} \quad (2.17)$$

When $V(\mathbf{r})$ depends on a single coordinate, all differential equations involved in constructing the Green function can be solved. Consider the case where V , F and T depend only on the radial coordinate, as happens in Section 3. Then the Green function satisfies the ordinary differential equation

$$Lg(r, r') = \frac{1}{r'^2} \delta(r - r'), \quad (2.18)$$

$$L = \frac{d^2}{dr^2} + 2 \left(\frac{1}{r} + \frac{dF}{dr} \right) \frac{d}{dr}.$$

Rather than expand in eigenfunctions, we construct g from the two solutions of $LR = 0$, which are known.

$$R^+(r) = 1; \quad R^-(r) = \int_{r_0}^r \frac{dr' e^{-2F(r')}}{r'^2}. \quad (2.19)$$

The Green function is

$$g(r, r') = R^+(r_>) R^-(r_<)/r'^2 W(r') = -R^+(r_>) R^-(r_<) e^{2F(r')}, \quad (2.20)$$

where W is the Wronskian

$$W(R^+, R^-) \equiv \frac{dR^+}{dr} R^- - R^+ \frac{dR^-}{dr} = -\frac{e^{-2F(r)}}{r^2}. \quad (2.21)$$

Now

$$T_n(r) = \int_0^\infty dr' r'^2 g(r, r') \left\{ \frac{2m}{\hbar^2} [V - E_n] \right. \quad (2.22)$$

$$\left. - F'' - \frac{2}{r'} F' - (F')^2 - (T'_{n-1})^2 \right\}_{r'}.$$

The eigenvalue equation emerges here, not through a zero mode, but through the bad asymptotic behavior of R^- . Near $r = 0$, $R^-(r) \sim e^{-2F(0)}/r$, and

$$T_n(r) \sim \frac{e^{-2F(0)}}{r} \int_0^\infty dr' r'^2 e^{2F(r')} \left\{ \frac{2m}{\hbar^2} [V - E_n] \right. \quad (2.23)$$

$$\left. - F'' - \frac{2}{r'} F' - (F')^2 - (T'_{n-1})^2 \right\}_{r'}.$$

To keep T_n finite at $r = 0$, the eigenvalue integral must vanish; when it does, $T_n(0) = 0$.

3 Spherical Square Well Potential

We begin our study of the anti-WKB approximation by applying it to the case of the spherically symmetric potential

$$V(r) = \begin{cases} -V_0 & (r < a); \\ 0 & (r > a). \end{cases} \quad (3.1)$$

The radial Schrödinger's equation for s-wave bound states can be solved, and the energies are determined by the equation[4]

$$ka \cot ka = -Ka; \quad ka = \sqrt{\frac{2ma^2}{\hbar^2} V_0 - (Ka)^2}; \quad E = -\frac{\hbar^2 K^2}{2m}. \quad (3.2)$$

There is no bound state unless V_0 exceeds the threshold strength

$$[V_0]_{thresh} = \frac{\hbar^2}{2ma^2} \left(\frac{\pi}{2}\right)^2 C_1; \quad C_1 = 1.0, \quad (3.3)$$

and for V_0 just above threshold strength, the energy of the ground state is

$$E = \frac{ma^2}{2\hbar^2} (V_0 - [V_0]_{thresh})^2 C_2; \quad C_2 = 1.0. \quad (3.4)$$

To compute E_0 we use the eigenvalue integral 2.23. To get some notion of the dependence of E_0 on the variational seed, we try three of them, each of which depends on a single parameter r_0 :

$$\begin{aligned} F_1(r) &= -Kr - \ln(r/r_0 + 1); \\ F_2(r) &= -Kr - \ln \sqrt{(r/r_0)^2 + 1}; \\ F_3(r) &= \begin{cases} 1 - (K + \frac{1}{r_0})r, & (r < r_0); \\ -Kr - \ln(r/r_0), & (r > r_0). \end{cases} \end{aligned} \quad (3.5)$$

(F_3 is chosen so that the function and its derivative are continuous at $r = r_0$.) Using these variational seeds, we obtain the results summarized in Table 2.1.

$F(r)$	r_0/a	C_1	C_2
$S(r)$ (exact)		1.0	1.0
$F_1(r)$	0.638	1.14	0.127
$F_2(r)$	0.923	1.09	1.37
$F_3(r)$	1.38	1.03	0.826

Table 2.1. The optimum values of r_0/a and the coefficients C_1 and C_2 for the three choices for $F(r)$.

Note that $E_0 = \mathcal{E}_0$ is a variational energy; in each case the parameter r_0/a has been chosen to minimize E_0 . We see that the results are sensitive to F . F_3 gives a threshold potential strength that is about 3% high, and it also gives the best estimate for the bound state energy near threshold. We use F_3 in the rest of Section 3.

To explore further we choose a potential strength well above threshold: $2ma^2V_0/\hbar^2 = 3.0$. The bound state energy is given by Eq. 3.2 to be $E = -0.0613\hbar^2/2ma^2$. We find that at this potential strength E_0 is minimized for $r_0/a = 1.505$ (in the threshold calculation the value was 1.37). We find $E_0 = -0.0379\hbar^2/2ma^2$. A measure of the (mediocre) quality of this result is the ratio $E_0/E = 0.619$.

We next compute E_1 . For this one degree-of-freedom problem, we use Eq. 2.2 because a simple formula for dT_n/dr is available:

$$\begin{aligned} \frac{dT_n}{dr} = \frac{e^{-2F(r)}}{r^2} \int_0^r dx x^2 e^{2F(x)} & \left\{ \frac{2m}{\hbar^2} [V(x) - E_n] \right. \\ & \left. - F''(x) - \frac{2}{x} F'(x) - [F'(x)]^2 - [T'_{n-1}(x)]^2 \right\}. \end{aligned} \quad (3.6)$$

We now obtain much improved results: $E_1 = -0.0589\hbar^2/2ma^2$, and $E_1/E = 0.960$. Almost 90% of the error in E_0 has been removed in E_1 .

One of the properties of the anti-WKB approximation we have emphasized is that it can be applied to potential problems where $V(\mathbf{r})$ has a general dependence on \mathbf{r} . This statement is qualified by the requirement that $F(\mathbf{r})$ be such that Eq. 2.9 can be solved for G . One case where this can be done is when V is *nearly* spherically symmetric. Then we choose F to depend on r , relying on the T_n to supply the nonspherical corrections. Note that the anti-WKB method is more flexible than the method of separation of coordinates in that it is not necessary for surfaces of constant potential to exactly fall on surfaces of constant coordinate. Approximate coincidence suffices. Below we use separation of coordinates to construct G in spherical coordinates.

When F depends only on r , we write G in the form

$$G(\mathbf{r}, \mathbf{r}') = \sum_{\ell=0}^{\infty} g_{\ell}(r, r') \sum_{m=-\ell}^{m=\ell} Y_{\ell m}(\theta, \phi) Y_{\ell m}^*(\theta', \phi'), \quad (3.7)$$

where the radial Green function satisfies

$$\frac{\partial^2 g_{\ell}(r, r')}{\partial r^2} + 2 \left(\frac{1}{r} + \frac{dF}{dr} \right) \frac{\partial g_{\ell}(r, r')}{\partial r} - \frac{\ell(\ell+1)}{r^2} g_{\ell}(r, r') = \frac{1}{r^2} \delta(r - r'). \quad (3.8)$$

This Green function is

$$g_{\ell}(r, r') = R_{\ell}^+(r_{>}) R_{\ell}^-(r_{<}) e^{2F(r')}/C_{\ell}, \quad (3.9)$$

where $R_{\ell}^{+,-}$ satisfy the homogeneous equation

$$\frac{d^2 R_{\ell}}{dr^2} + 2 \left(\frac{1}{r} + \frac{dF}{dr} \right) \frac{dR_{\ell}}{dr} - \frac{\ell(\ell+1)}{r^2} R_{\ell} = 0. \quad (3.10)$$

The factor C_{ℓ} comes from the Wronskian $W(R_{\ell}^+, R_{\ell}^-) = C_{\ell} e^{-2F(r)}/r^2$.

For $\ell = 0$, Eq. 3.10 has the same solutions we found for the case of spherical symmetry, and we can choose $R_0^{+,-} = R^{+,-}$ of Eq. 2.19. We again encounter the eigenvalue integral 2.23 with this change: Only the s -wave projection of V enters into the determination of E_0 . This is in keeping with our assumption that V is nearly spherically symmetric. The higher E_n 's receive contributions from all of the angular projections of V .

The solutions of Eq. 3.10 for $\ell > 0$ require further analysis. We first note that near $r = 0$ they behave like r^{ℓ} or $r^{-\ell-1}$, and we must choose R_{ℓ}^- to have the nonsingular behavior r^{ℓ} . At large r , solutions of Eq. 3.10 behave like

those of Eq. 2.19 because the last term in Eq. 3.10 is unimportant at large r . We must choose the solution behaving like a constant so that R^+ remains finite at large r .

In the case of $F_3(r)$, Eq. 3.10 has solutions that are familiar functions. In the interval $r < r_0$, these are confluent hypergeometric functions:

$$\begin{aligned} R_{\ell 1} &= r^\ell \Phi(\ell, 2\ell + 2, 2Kr + 2r/r_0), \\ R_{\ell 2} &= r^{-\ell-1} \Phi(-\ell - 1, -2\ell, 2Kr + 2r/r_0). \end{aligned} \quad (3.11)$$

In the interval $r > r_0$ they are modified spherical Bessel functions:

$$R_{\ell 3} = \sqrt{r} e^{Kr} I_{\ell+1/2}(Kr), \quad R_{\ell 4} = \sqrt{r} e^{Kr} K_{\ell+1/2}(Kr). \quad (3.12)$$

We then have the solutions

$$R_\ell^- = \begin{cases} R_{\ell 1}, & r < r_0; \\ \alpha R_{\ell 3} + \beta R_{\ell 4}, & r > r_0; \end{cases} \quad R_\ell^+ = \begin{cases} \gamma R_{\ell 1} + \delta R_{\ell 2}, & r < r_0; \\ R_{\ell 4}, & r > r_0. \end{cases} \quad (3.13)$$

The coefficients are fixed by demanding that the functions and their first derivatives be continuous at $r = r_0$; they may be expressed in terms of Wronskians evaluated at $r = r_0$.

When a particle moves under the influence of a highly nonspherical potential, the Green function should be constructed in coordinates chosen so it is reasonable for F to depend only on one of them, ξ . As an example, consider a potential well in the shape of a right circular cylinder of diameter D and length L :

$$V(\mathbf{r}) = \begin{cases} -V_0 & |z| < L/2, \sqrt{x^2 + y^2} < D/2; \\ 0 & \text{otherwise.} \end{cases} \quad (3.14)$$

If $L \sim D$, this is an example of an approximately spherical potential, and it is appropriate to use the Green function constructed above. Here we consider the case of a long thin rod: $L \gg D$. Now it is manifestly inadequate to take the surfaces of constant F to be spherical. These surfaces ought to be figures of rotation about the z -axis in the form of elongated cigars: prolate spheroids. This suggests use of the prolate spheroidal coordinate system:

$$\begin{aligned}
x &= \frac{r_0}{2} \sqrt{\xi^2 - 1} \sin \theta \cos \phi, \\
y &= \frac{r_0}{2} \sqrt{\xi^2 - 1} \sin \theta \sin \phi, \\
z &= \frac{r_0}{2} \xi \cos \theta; \\
1 \leq \xi < \infty, \quad 0 \leq \theta \leq \pi, \quad 0 \leq \phi < 2\pi; \\
dV &= \left(\frac{r_0}{2}\right)^3 (\xi^2 - \cos^2 \theta) \sin \theta d\xi d\theta d\phi.
\end{aligned} \tag{3.15}$$

Surfaces of constant ξ are ellipsoids of revolution about the z-axis, the ellipses having foci at $z = \pm r_0/2$. If r_0 is appropriately chosen (by a variational minimization of E_0), the shape of the ellipsoids can be made to resemble that of the rod for $\xi \sim 1$; for large ξ the ellipsoids approach spheres of radius $r_0\xi/2$. An obvious choice for F is

$$F(\xi) = -Kr_0\xi/2 - \ln \xi. \tag{3.16}$$

In prolate spheroidal coordinates, Eq. 2.9 takes the form

$$\begin{aligned}
&\frac{\partial}{\partial \xi} \left[(\xi^2 - 1) \frac{\partial G}{\partial \xi} \right] + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left[\sin \theta \frac{\partial G}{\partial \theta} \right] + \left[\frac{1}{\xi^2 - 1} + \frac{1}{\sin^2 \theta} \right] \frac{\partial^2 G}{\partial \phi^2} \\
&+ 2(\xi^2 - 1) \frac{dF}{d\xi} \frac{\partial G}{\partial \xi} = \frac{2}{r_0} \delta(\xi - \xi') \delta(\cos \theta - \cos \theta') \delta(\phi - \phi').
\end{aligned} \tag{3.17}$$

The solution has the form

$$G(\xi, \theta, \phi; \xi', \theta', \phi') = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} g_{\ell,m}(\xi, \xi') Y_{\ell m}(\theta, \phi) Y_{\ell m}^*(\theta', \phi'), \tag{3.18}$$

where the radial Green function satisfies

$$\begin{aligned}
(\xi^2 - 1) \frac{\partial^2 g_{\ell m}}{\partial \xi^2} + 2 \left[\xi + (\xi^2 - 1) \frac{dF}{d\xi} \right] \frac{\partial g_{\ell m}}{\partial \xi} - \left[\ell(\ell + 1) + \frac{m^2}{\xi^2 - 1} \right] g_{\ell m} \\
= \frac{2}{r_0} \delta(\xi - \xi').
\end{aligned} \tag{3.19}$$

The radial Green function is

$$g_{\ell m}(\xi, \xi') = \frac{2}{r_0 C_{\ell m}} e^{2F(\xi')} \Xi_{\ell m}^-(\xi_{<}) \Xi_{\ell m}^+(\xi_{>}). \tag{3.20}$$

$C_{\ell m}$ appears in the Wronskian $W(\Xi^+, \Xi^-) = C_{\ell m} e^{-2F}/(\xi^2 - 1)$. The functions $\Xi_{\ell m}^\pm$ satisfy the homogeneous equation obtained by removing the delta function source in Eq. 3.19.

The general method of constructing the Green function appropriate to the rod-shaped potential well is now clear. We discontinue discussion of the functions $\Xi_{\ell m}^\pm$ except to point out that the differential equation they satisfy has three regular singular points and an irregular singular point at infinity.

4 Long Range Potentials

When a potential is long range and behaves at large distance like r^{-p} , $1 < p < 2$, there is no longer a threshold strength for the bound state.[5] The anti-WKB approximation reproduces this result, and it does so in lowest order, when $n = 0$. We demonstrate this by showing that with the choices of F given by Eq. 3.5 we can adjust r_0 so that $E_0=0$ no matter how weak the strength of the potential tail. A further adjustment of r_0 will then produce a negative (bound state) energy.

We consider the case of F_2 . For the potential V_0/r^p , ($r > a$), the eigenvalue equation implied by Eq. 2.23 takes the form, when $n = E_0 = 0$:

$$0 = -\frac{2mV_0}{\hbar^2} \int_a^\infty \frac{r^{2-p} dr}{r^2 + r_0^2} + 3r_0^2 \int_0^\infty \frac{r^2 dr}{(r^2 + r_0^2)^3}. \quad (4.1)$$

This may be written

$$0 = -\frac{mV_0 r_0^{1-p}}{\hbar^2} \frac{2\pi}{2 \sin \pi(p-1)/2} - \sum_{k=0}^{\infty} \left(\frac{a}{r_0} \right)^{2k+3-p} \frac{(-1)^k}{k + (3-p)/2} + \frac{3\pi}{16r_0}. \quad (4.2)$$

For $1 < p < 2$, there is some large value of r_0 for which this equation is satisfied, no matter how small V_0 may be. There must be a nodeless bound state.

When $p = 1$, we come to the classic case of the Coulomb potential. At this point, the asymptotic behavior of the wavefunction changes, and in three dimensions the coefficient of the $\ln(r/r_0)$ term depends on the potential strength and bound state energy. Since this coefficient is no longer known, the obvious response is to treat this coefficient as an additional parameter,

r_1 . Thus, for example, F_3 is generalized to

$$F_3(r) = \begin{cases} r_1 - (K + \frac{r_1}{r_0})r, & (r < r_0); \\ -Kr - r_1 \ln(r/r_0), & (r > r_0). \end{cases} \quad (4.3)$$

But now the determination of the variational parameters is obvious, because with $r_1 = 0$, $F_3 = -Kr = S$. Therefore $T(r) = 0$, and we immediately have the hydrogen wavefunction, with $E_0 = E$. The same result is achieved with F_1 and F_2 .

It is fortuitous that the hydrogen wavefunction occurs among the natural choices for F . Still, it is nice that the Coulomb potential is so easily encompassed by the anti-WKB approximation.

5 ϕ^4 Field Theory

The anti-WKB approximation can be applied to problems having many degrees of freedom. We illustrate this using the case of ϕ^4 field theory in one spatial dimension. In the continuum the Hamiltonian is

$$H = \int_0^L dx \left\{ \frac{1}{2} c^2 \pi^2(x) + \frac{1}{2} \left[\frac{d\phi(x)}{dx} \right]^2 + \frac{1}{2} \frac{c^2}{\hbar^2} (m^2 + \delta m^2) \phi^2(x) + \frac{\lambda}{24} \phi^4(x) \right\}. \quad (5.1)$$

We identify fields at $x = 0$ and $x = L$. To treat the system by the anti-WKB method we must deal with a discrete set of degrees of freedom. We therefore divide the line into N segments of length a ; $N = L/a$. Each segment is represented by a dimensionless lattice coordinate ϕ_k , $k = 1, \dots, N$. The lattice Hamiltonian is

$$H = \frac{\hbar c}{a} \sum_{k=1}^N \left[-\frac{1}{2} \frac{\partial^2}{\partial \phi_k^2} + \frac{1}{2} (\phi_{k+1} - \phi_k)^2 + \frac{1}{2} \left(\frac{ca}{\hbar} \right)^2 (m^2 + \delta m^2) \phi_k^2 + \frac{\lambda \hbar ca}{24} \phi_k^4 \right]. \quad (5.2)$$

Putting the field theory on the lattice introduces a short distance cutoff a , or equivalently a large momentum cutoff \hbar/a . This removes the notorious

divergences of continuum quantum field theory. However, the divergences still lurk and reveal themselves when we approach the continuum limit by taking $a \rightarrow 0$, $N \rightarrow \infty$, with $Na = L$ fixed. We want to be able to take the limit, of course, since for us the lattice is only a computational device. In our case we find that as we take $a \rightarrow 0$ we approach a continuum theory having infinite mass. (We show this below.) This pathology disappears when we include an appropriate mass counterterm in the Hamiltonian:

$$\delta m^2 = -\frac{\lambda \hbar}{4c} \Delta_0; \quad \Delta_0 = \frac{1}{N} \sum_{p=1}^N \frac{1}{\omega_0(p)}; \quad (5.3)$$

$$\omega_0(p) = \sqrt{\left(\frac{mca}{\hbar}\right)^2 + 4 \sin^2\left(\frac{\pi p}{N}\right)}.$$

This counterterm is the lattice version of the very counterterm that must be included in the continuum Hamiltonian. At small a , Δ_0 grows logarithmically to keep the effective mass finite.

$$\Delta_0 \sim \frac{1}{\pi} \ln \frac{\hbar^2}{m^2 c^2 a^2}. \quad (5.4)$$

In one spatial dimension ϕ^4 field theory is superrenormalizable. [6] For this system, the explicit counterterm in 5.3 suffices to remove all $a \rightarrow 0$ divergences in “physical” entities like the correlator

$$\langle 0 | \phi(0) \phi(x) | 0 \rangle \sim \hbar c \langle 0 | \frac{1}{N} \sum_{k=1}^N \phi_k \phi_{k+x/a} | 0 \rangle. \quad (5.5)$$

Unfortunately, the groundstate energy E that has figured prominently in the anti-WKB approximation is not “physical” in the sense used here. Even free field theory, $\lambda = 0$, includes zero point energies for each degree of freedom, and when summed these diverge as $a \rightarrow 0$. We will cope with E as we go along. This point aside, Eqs. 5.2, 5.3 define a lattice representation of continuum ϕ^4 field theory to which we can apply the anti-WKB approximation.

A central issue for this many degree of freedom problem is finding an F that is appropriate, and for which the multidimensional integrals and Green function can be found. There is just one choice for which this is *easy*:

$$F = -\frac{1}{2} \sum_{k_1 k_2} M_{k_1 k_2} \phi_{k_1} \phi_{k_2} \equiv -\frac{1}{2} \phi M \phi, \quad (5.6)$$

with M a real symmetric matrix. Consider the eigenvalue equation for E_0 .

$$0 = \int (\Pi d\phi) e^{-\phi M \phi} \left\{ \sum_k \left[(\phi_{k+1} - \phi_k)^2 + (ca/\hbar)^2 (m^2 + \delta m^2) \phi_k^2 + (\lambda \hbar c a^2) \phi_k^4 / 12 \right] - 2E_0 a / \hbar c + Tr(M) - \phi M^2 \phi \right\}. \quad (5.7)$$

Every term in the brace involves powers of ϕ_k , so the integral can be evaluated by taking derivatives with respect of α_k of the generating function

$$I_1(\alpha) = \int (\Pi d\phi) \exp(-\phi M \phi + i \alpha \phi); \quad \alpha \phi \equiv \sum_k \alpha_k \phi_k. \quad (5.8)$$

This generator, in turn, can be evaluated easily by a change of coordinates. Let the eigenvectors and eigenvalues of M be v^q and μ^q .

$$M v^q = \mu^q v^q, \quad (q = 1, \dots, N). \quad (5.9)$$

The new coordinates are

$$\eta^q = \sum_k \phi_k v_k^q; \quad \phi_k = \sum_q \eta^q v_k^q. \quad (5.10)$$

In these coordinates I_1 becomes a product of N independent Gaussian integrals, and

$$I_1(\alpha) = \frac{\pi^{N/2}}{\sqrt{\det M}} \exp \left(-\frac{1}{4} \alpha M^{-1} \alpha \right). \quad (5.11)$$

Eq. 5.7 becomes

$$0 = I_1(0) \left\{ \sum_k \left[M_{kk}^{-1} - M_{k,k+1}^{-1} + (ca/\hbar)^2 (m^2 + \delta m^2) M_{kk}^{-1} / 2 + (\lambda \hbar c a^2) (M_{kk}^{-1})^2 / 16 \right] - 2E_0 a / \hbar c + Tr(M) - Tr(M^2 M^{-1}) \right\}. \quad (5.12)$$

$M_{k_1 k_2}$ must be a function of $k_1 - k_2$ of period N owing to the homogeneity and periodicity of the Hamiltonian. It can be written as a discrete Fourier transform.

$$M_{k_1 k_2}^{\pm 1} = \frac{1}{N} \sum_{p=1}^N \omega^{\pm 1}(p) \exp \left[\frac{2\pi i p (k_1 - k_2)}{N} \right]. \quad (5.13)$$

With this the eigenvalue equation decouples into modes.

$$0 = I_1(0) \left\{ \sum_p \left[\frac{\omega(p)}{2} + \frac{1}{\omega(p)} \left(1 - \cos \frac{2\pi p}{N} + (ca/\hbar)^2 (m^2 + \delta m^2) \right) \right] + N(\lambda \hbar c a^2) \left[\frac{1}{N} \sum_p \frac{1}{\omega(p)} \right]^2 - \frac{2E_0 a}{\hbar c} \right\}. \quad (5.14)$$

The $\omega(p)$ are parameters in M that are fixed by minimizing E_0 . We find

$$\omega(p) = \sqrt{\left(\frac{ca}{\hbar}\right)^2 (m^2 + \delta m^2) + \frac{\lambda \hbar c a^2}{4} \Delta + \sin^2 \left(\frac{\pi p}{N}\right)}, \quad (5.15)$$

$$\Delta = \frac{1}{N} \sum_p \frac{1}{\omega(p)}. \quad (5.16)$$

Eq. 5.16 determines Δ , and it is enlightening to examine its solution near the continuum limit *when we drop the counterterm* δm^2 . Following Eq. 5.4,

$$\Delta \sim \frac{1}{\pi} \ln \frac{4}{\lambda \hbar c a^2 \Delta}; \quad \Delta \sim \frac{1}{\pi} \ln \frac{4}{\lambda \hbar c a^2} + O\left(\ln \ln \frac{4}{\lambda \hbar c a^2}\right). \quad (5.17)$$

Therefore, the square of the effective mass in $\omega(p)$ becomes, in the limit of small a ,

$$m^2 + \frac{\lambda \hbar^3 \Delta}{4c} \sim m^2 + \frac{\lambda \hbar^3}{4\pi c} \ln \frac{4}{\lambda \hbar c a^2}. \quad (5.18)$$

This shows that we approach a continuum theory having infinite mass. On the other hand, when we do include the counterterm, Eq. 5.16 has the solution $\Delta = \Delta_0$; $\omega(p) = \omega_0(p)$. Then the mode function $\omega(p)$ never changes, no matter what the lattice spacing or coupling strength.

The energy E_0 is

$$\frac{E_0}{L} = \frac{\hbar c}{2a^2} \left[\frac{1}{N} \sum_{p=1}^N \omega(p) \right] - \frac{m^2 c^3}{\hbar} \left(\frac{\lambda \hbar^3}{m^2 c} \right) \Delta_0^2. \quad (5.19)$$

The sum on the right is the zero-point energy of the degrees of freedom. It is present in free field theory, and its contribution is quadratically divergent in a^{-1} . The last term, proportional to the dimensionless coupling $\lambda \hbar^3 / m^2 c$, diverges like $(\ln a^{-1})^2$. In perturbation theory it arises because anomalous

combinatorics spoil the cancellation of divergences in self-energy loops and Δ_0 . This failure to cancel occurs only at order λ of perturbation theory, so E_0 already exhibits all the terms that diverge as $a \rightarrow 0$.

To compute E_1 we need the Green function satisfying

$$\left(\frac{\partial^2}{\partial \phi^2} - 2\phi M \frac{\partial}{\partial \phi} \right) G(\phi, \phi') = \prod_k \delta(\phi_k - \phi'_k), \quad (5.20)$$

in matrix notation. We use Eq. 2.12 to construct G , which requires us to construct eigenfunctions of the operator on the left. We again use coordinates η ; then the equation for the eigenfunctions and eigenvalue is

$$\sum_{q=1}^N \left[\frac{\partial^2}{\partial (\eta^q)^2} - 2\mu^q \eta^q \frac{\partial}{\partial \eta^q} \right] \psi = \mu \psi. \quad (5.21)$$

This equation may be solved by separation of variables.

$$\psi_{\{s\}} = \prod_{q=1}^N H_{s_q}(\eta^q \sqrt{\mu^q}). \quad (5.22)$$

The functions H_s are Hermite polynomials satisfying

$$\begin{aligned} \frac{d^2 H_s(x)}{dx^2} - 2x \frac{dH_s(x)}{dx} + 2s H_s(x) &= 0, \\ \int_{-\infty}^{\infty} dx e^{-x^2} H_{s_1}(x) H_{s_2}(x) &= \delta_{s_1, s_2} \sqrt{\pi} 2^{s_1} (s_1!). \end{aligned} \quad (5.23)$$

There are N indices on our wave function, and the eigenvalue is a linear function of them:

$$\mu = -2 \sum_{q=1}^N s_q \mu^q. \quad (5.24)$$

The Green function is

$$\begin{aligned} G = \left(-\frac{1}{2} \right) e^{-\phi' M \phi'} \int_0^1 \frac{dz}{z} \prod_{q=1}^N \sqrt{\frac{\mu_q}{\pi}} \left[\sum_{s_q=0}^{\infty} \left(\frac{z^{\mu_q}}{2} \right)^{s_q} \right. \\ \left. \times \frac{H_{s_q}(\eta^q \sqrt{\mu^q}) H_{s_q}(\eta^{q'} \sqrt{\mu^q})}{(s_q!)} \right]. \end{aligned} \quad (5.25)$$

The purpose of the integration over z is to produce the denominator $1/\mu_k$ in Eq. 2.12. The sum over s_q is given by Mehler's formula. [7] Reverting to the original variables,

$$G(\phi, \phi') = -\frac{1}{2} \frac{\sqrt{\det(M)}}{\pi^{N/2}} \int_{\epsilon}^1 \frac{dz}{z \sqrt{\det(1 - z^{2M})}} \exp \left[-\phi' \frac{M}{1 - z^{2M}} \phi' - \phi \frac{M z^{2M}}{1 - z^{2M}} \phi + 2\phi' \frac{M z^M}{1 - z^{2M}} \phi \right]. \quad (5.26)$$

As we expect from the discussion of Section 2, this Green function does not exist because $\mu = 0$ is an eigenvalue. In Eq. 5.26 the divergence appears at $z = 0$, and it has been regulated by a cutoff at $z = \epsilon$. However, when computing T_n , the coefficient of the $1/z$ factor is

$$D = \left\{ \sum_k \left[(\phi_{k+1} - \phi_k)^2 + \left(\frac{ca}{\hbar} \right)^2 (m^2 + \delta m^2) \phi_k^2 + \frac{\lambda \hbar c a^2}{12} \phi_k^4 \right] - \frac{2aE_n}{\hbar c} + \text{Tr}(M) - \phi M^2 \phi - \left(\frac{\partial T_{n-1}}{\partial \phi} \right)^2 \right\}. \quad (5.27)$$

Setting this to zero, we obtain a finite T_n as $\epsilon \rightarrow 0$. Thus we again encounter the eigenvalue equation as a consistency condition for the solution of Schrödinger's equation.

The dependencies on the fields in Eq. 5.26 are Gaussian, so we can use I_1 to evaluate the generating function

$$\begin{aligned} I_2(\alpha, \beta) &= \int (\prod d\phi d\phi') G(\phi, \phi') \exp(-\phi M \phi + i\alpha \phi + i\beta \phi') \\ &= \frac{\pi^{N/2}}{\sqrt{\det(M)}} \exp \left(-\frac{1}{4} \alpha M^{-1} \alpha - \frac{1}{4} \beta M^{-1} \beta \right) \\ &\quad \times \left(-\frac{1}{2} \right) \int_{\epsilon}^1 \frac{dz}{z} \exp \left(-\frac{1}{2} \alpha [z^M M^{-1}] \beta \right). \end{aligned} \quad (5.28)$$

By differentiation of I_2 we obtain all the contributions in

$$E_1 - E_0 = \frac{\hbar c}{2a} \frac{\int (\prod d\phi d\phi') e^{-\phi M \phi} G(\phi, \phi') D(\phi) D(\phi')}{\int (\prod d\phi) e^{-\phi M \phi}}. \quad (5.29)$$

The result is

$$\frac{E_1 - E_0}{L} = -\frac{m^2 c^3}{\hbar} \left(\frac{\lambda \hbar^3}{m^2 c} \right)^2 \frac{\Delta_2}{384}, \quad (5.30)$$

where

$$\Delta_2 = \left(\frac{mca}{\hbar} \right)^2 \int_0^1 \frac{dz}{z} \frac{1}{N} \left[\sum_{k_1, k_2} \left(z^M M^{-1} \right)_{k_1, k_2} \right]^4. \quad (5.31)$$

Using Eq. 5.13,

$$(z^M M^{-1})_{k_1, k_2} = \frac{1}{n} \sum_{p=1}^N \frac{z^{\omega_0(p)}}{\omega_0(p)} \exp \left[\frac{2\pi i p(k_1 - k_2)}{N} \right], \quad (5.32)$$

$$\begin{aligned} \Delta_2 &= \left(\frac{mca}{\hbar} \right)^2 \left(\frac{1}{N} \right)^3 \sum_{p_1, p_2, p_3} \frac{1}{\omega_0(p_1)\omega_0(p_2)\omega_0(p_3)\omega_0(p_1 + p_2 + p_3)} \\ &\quad \times \frac{1}{[\omega_0(p_1) + \omega_0(p_2) + \omega_0(p_3) + \omega_0(p_1 + p_2 + p_3)]}. \end{aligned} \quad (5.33)$$

It is straightforward to verify that Δ_2 remains finite as $a \rightarrow 0$.

What emerges after all our work appears to be perturbation theory in “old-fashioned” form. This is easily demonstrated. We have $E_1 - E_0 = O(\lambda^2) = O[(\partial T_0 / \partial \phi)^2]$. Hence, $T_0 = O(\lambda)$. Then use

$$\begin{aligned} T_n - T_{n-1} &= \int (\Pi d\phi') G(\phi, \phi') \left[\frac{2a}{\hbar c} (E_{n-1} - E_n) \right. \\ &\quad \left. + \left(\frac{\partial T_{n-2}}{\partial \phi} \right)^2 - \left(\frac{\partial T_{n-1}}{\partial \phi} \right)^2 \right], \quad (5.34) \\ E_n - E_{n-1} &= \frac{\int (\Pi d\phi) e^{2F} [(\partial T_{n-2} / \partial \phi)^2 - (\partial T_{n-1} / \partial \phi)^2]}{\int (\Pi d\phi) e^{2F}} \end{aligned}$$

to prove by induction $T_n - T_{n-1} = O(\lambda^{n+1}) = E_n - E_{n-1}$. This result is not surprising. Our F is the S of free field theory, and we compute corrections to that. This is the program of perturbations theory.

No one wants to use the anti-WKB approximation to develop perturbation theory. What we learn from our exercise is that the calculations can be

carried out, and they lead to a sensible and familiar result. But it is possible, within the anti-WKB approximation, to contemplate alternatives that transcend perturbation theory. An obvious generalization of F is

$$\tilde{F} = \sum_{q=1}^N \left[-\frac{1}{2} \tilde{\mu}^q (\eta^q)^2 - \frac{1}{4} \tilde{\nu}^q (\eta^q)^4 \right]. \quad (5.35)$$

We use plane wave coordinates so that all degrees of freedom are coupled. The mode eigenvalue equation is unfamiliar, and Mehler's formula is not available, so we must work harder. A computer would be required to assemble G .

A payoff is possible when a seed like \tilde{F} is used. Recall that at $\lambda \hbar^3 / m^2 c \sim 10$, ϕ^4 field theory makes a transition to a state of broken $\phi \leftrightarrow -\phi$ symmetry in which the field has a vacuum expectation value: $\langle 0 | \phi(x) | 0 \rangle = \phi_0 \neq 0$. [6] From this fact alone we see that F must be inadequate at strong coupling because with F , $\phi_0 = 0$. But in \tilde{F} , as the variational parameters $\tilde{\mu}^q$ vary smoothly with λ , a vacuum expectation value can develop beyond a critical coupling.

A trick attributed to Feynman applies to this problem. Extend H by adding a term $\xi(1/N) \sum_k \phi_k \phi_{k+d}$. The extended Hamiltonian remains homogeneous and periodic, so the techniques we have developed continue to apply. E depends on ξ , of course, and by first order perturbation theory (in ξ), $dE/d\xi(\xi=0)$ is just the correlator of Eq. 5.5. In this formula we would substitute E_n for E .

6 Helium

Because of the Pauli principle, helium is the only multi-electron atom in which a symmetric spatial wave function is physical. The nodeless state we construct is the groundstate of helium.

The Hamiltonian we study includes only the potential terms representing the electric forces acting on electrons moving around an immobile nucleus. The ground state energy of the simplified Hamiltonian therefore differs slightly from that of physical helium where magnetic, recoil and relativistic corrections are present. The Hamiltonian is

$$H = -\frac{1}{2}(\nabla_1^2 + \nabla_2^2) - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}. \quad (6.1)$$

We use dimensionless coordinates, so the eigenvalues of H must be multiplied by me^4/\hbar^2 .

A standard textbook variational computation with this Hamiltonian assumes that the wavefunction is a product of exponential (hydrogenic) factors. [8] The resulting energy, $\langle H \rangle = -(27/16)^2 = -2.848$, is very close to the experimental groundstate energy, -2.90, and we adopt it as a standard for the problem. Since we have the tools to deal with many-body problems when F is a quadratic form, we use that:

$$F = -\frac{1}{2}K_0(r_1^2 + r_2^2) - K_1\mathbf{r}_1 \cdot \mathbf{r}_2. \quad (6.2)$$

Our choice of F corresponds to a Gaussian first guess for the helium wavefunction. We compute E_0 , choosing K_0 and K_1 to minimize it and find

$$E_0 = -2.324; \quad K_0 = 1.549 \quad K_1 = (0.09238)K_0. \quad (6.3)$$

We obtain only 0.816 of the “standard” binding, which means that the anti-WKB correction is substantial.

An interesting feature of our result is that K_1 is so small. The repulsion between electrons enhances the probability of finding the electrons on opposite sides of the nucleus, but not by much. In fact, if we set $K_1 = 0$, the binding is decreased by less than 1%, and $E_0 = -2.301$. We use this version of F when calculating E_1 because of the resulting simplifications. The computation of E_1 now parallels that of Section 5. The main new feature is that the terms in the potential are Coulomb, not polynomial. When we use generating function I_2 , we integrate over parameters to generate the Coulomb terms, using the relation

$$\frac{1}{r} = \frac{1}{2\pi^2} \int \frac{d^3\alpha}{\alpha^2} \exp[i\alpha \cdot \mathbf{r}]. \quad (6.4)$$

Summarizing our results:

$$\begin{aligned} E_0 = -2.301; \quad E_1 = -2.707, \quad \langle H \rangle = -2.848; \\ \frac{E_0}{\langle H \rangle} = 0.808, \quad \frac{E_1}{\langle H \rangle} = 0.951. \end{aligned} \quad (6.5)$$

7 Conclusions

We have proposed an approximation for quantum mechanics and field theory that assumes the relative importance of gradient and Laplacian terms is the reverse of that in the WKB approximation. As with any such scheme, usefulness is an important issue. We have explored usefulness by applying the anti-WKB approximation to several problems. The examples of the spherical square well and the helium atom provide interesting numerical results. In these cases we chose a simple variational seed F and found that the initial (variational) estimates of the ground state energy were incorrect by several tens of percent. The first nontrivial anti-WKB correction removed three quarters of the error, or more.

In practice, the WKB method is difficult to apply to problems with many degrees of freedom. The anti-WKB method does suffer from this fault. With a quadratic choice for F we developed the formulas necessary for the treatment of the rather different problems of ϕ^4 field theory and the helium atom.

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References

- [1] L. D. Landau and E. M. Lifschitz, *Quantum Mechanics, Non-Relativistic Theory*, 2nd ed. (Pergamon, N. Y., 1965), pp. 158-187.
- [2] J. B. Bronzan, *Am. J. Phys.*, **55**: 54, 1987.
- [3] L. D. Landau and E. M. Lifschitz, *op. cit.*, pp. 58-60.
- [4] *ibid.*, p. 109.
- [5] *ibid.*, pp. 54-55.
- [6] S.-J. Chang *Phys. Rev D***10**: 2778, 1976.
- [7] H. Bateman, *Higher Transcendental Functions* (Mc Graw Hill, N. Y., 1955), V. 2, p. 194.
- [8] L. D. Landau and E. M. Lifschitz, *op. cit.*, pp. 239-240.